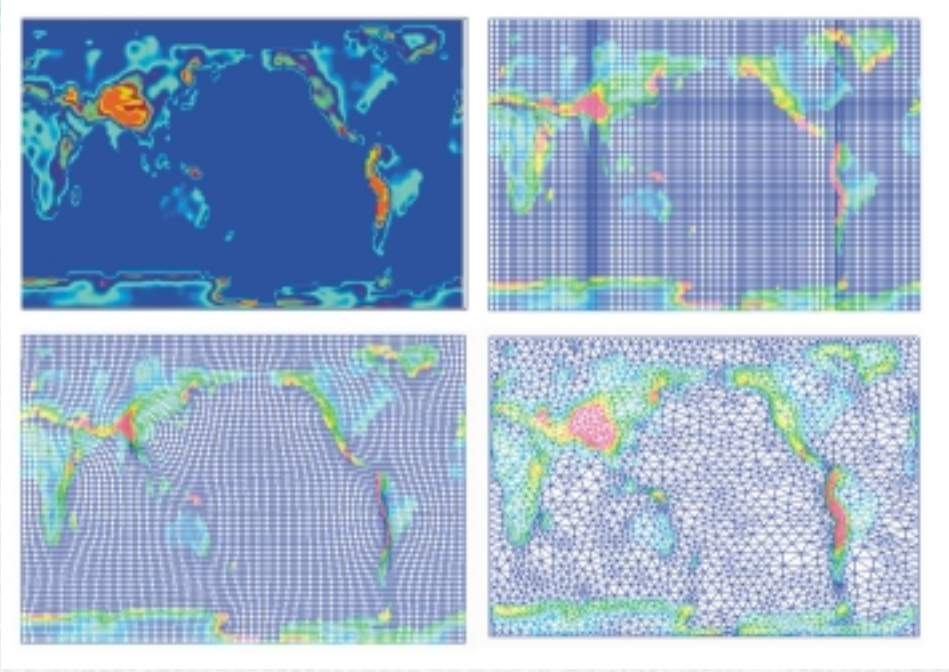
# Terascale Simulation Tools and Technology Center

## Vision

Terascale computing provides an unprecedented opportunity to achieve numerical simulations at levels of detail and accuracy previously unattainable. The Terascale Simulation Tools and Technology (TSTT) Center enables scientists to perform such simulations by enabling them to more easily use modern high-order, adaptive, parallel mesh and discretization tools. TSTT researchers work directly with a number of Scientific Discovery through Advanced Computing (SciDAC) application teams to introduce these new technologies into their application domains. The TSTT Center is also creating new technology that eases the use of such tools, not only for SciDAC applications, but also across a broad range of application areas that require mesh and discretization tools for scientific simulation. The TSTT partners, representing six U.S. Department of Energy (DOE) national laboratories and two universities, bring extensive expertise in structured, unstructured, and hybrid meshing and discretization technologies into one center with the goal of delivering advanced, mesh-based simulation capabilities to scientific applications in support of the DOE Office of Science mission. Through a five-year program to deliver technology to applications, and to create common interfaces that will allow multiple meshing and discretization technologies to interoperate, TSTT will eliminate the technical and human barriers preventing the effective use of powerful meshing and discretization techniques in large-scale scientific simulations.



*Plug-and-play access to multiple mesh and discretization technologies will allow application scientists to rapidly evaluate different methodologies.*

## TSTT Center Software

TSTT's research will be encapsulated into software components with well-defined interfaces that enable different mesh types, discretization strategies, and adaptive techniques to interoperate in a "plug and play" fashion. The interface design is driven by application scientists' requirements and the need for intuitive, easy-to-use interfaces at multiple levels of sophistication. All software developed as part of the TSTT Center will be freely available in the public domain. To ensure the relevance of our research and software developments to SciDAC goals, we collaborate closely with both SciDAC application researchers and other software infrastructure centers.

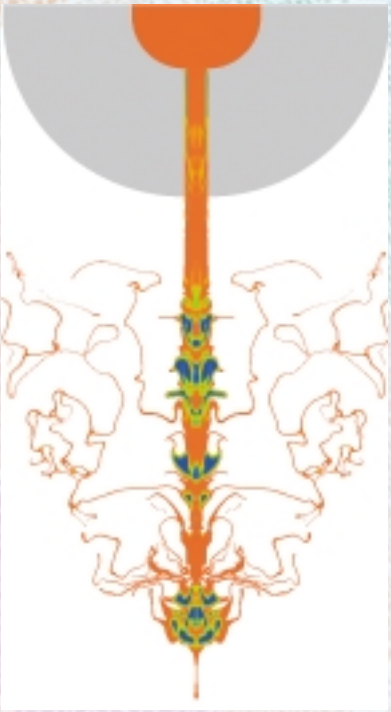
## TSTT and the SciDAC Application Teams

- *Accelerator Design:* TSTT is helping to improve stability of time-dependent electromagnetic codes by understanding the dependence of simulation code stability on mesh quality, and by improving the stability properties of the discretization algorithms. TSTT mesh-generation technology is being used to shorten the time required to generate high-quality meshes.
- *Astrophysics:* TSTT has demonstrated the potential impact of high-order Discontinuous Galerkin discretization methods for hydrodyamics and neutrino transport. These methods can improve accuracy and reduce time to solution for astrophysics applications.
- *Climate:* TSTT has investigated mesh generation strategies that create high-quality meshes with vertices focused over regions of high altitude. TSTT and the members of the climate modeling community have jointly developed a new preconditioner for spectral element simulations, accelerating the solution of a test problem based on shallow water equations.
- *Diesel spray formation:* TSTT is applying advanced front-tracking technology to create a simulation code modeling spray formation in diesel jet breakup.
- *Fusion:* TSTT is investigating the use of high-order adaptive finite element methods to improve the performance of MHD fusion simulations.
- *Computational biology:* TSTT is applying meshing technology in a novel way to develop image reconstruction and feature extraction for complex biological systems.

## TSTT and the SciDAC Integrated Software Infrastructure Centers

*Center for Component Technology for Terascale Simulation Software (CCTTSS):* TSTT is working to incorporate CCTTSS technology into TSTT software and to ensure compatibility between the software produced by the two centers.

*Terascale Optimal PDE Simulations Center (TOPS):* TSTT has incorporated the PETSc solver software into TSTT discretization frameworks. TSTT is carefully following the definition of TOPS vector, matrix, and solver interfaces to ensure compatibility between TOPS and TSTT software.



*TSTT front-tracking technology is used to understand the breakup of diesel jets into droplets.*

*Performance Center (PERC):* TSTT will use software from the ROSE project to optimize performance of the TSTT discretization library.

*Applied Partial Differential Equations Center (APDEC):* TSTT is working with APDEC to provide mesh interfaces for embedded boundary meshes that will be compatible with TSTT meshing interfaces.

## The TSTT Team

The TSTT team consists of researchers from six DOE national laboratories (ANL, LLNL, BNL, SNL, PNNL, and ORNL) and two universities (Rensselaer Polytechnic Institute and SUNY Stony Brook).

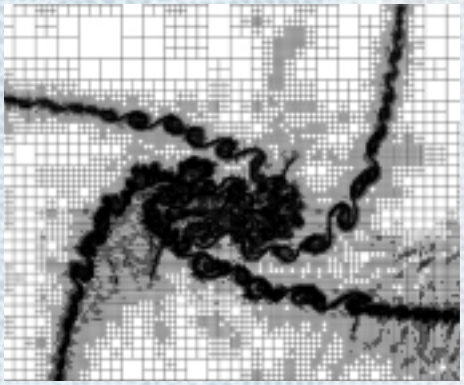
*More information about the TSTT center can be obtained by visiting http://tstt-scidac.org/*

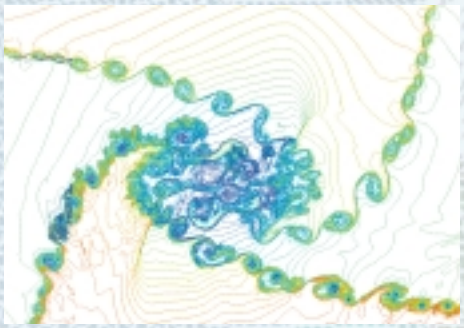

Contacts

*David L. Brown, LLNL, (925) 424-3557, dlb@llnl.gov*

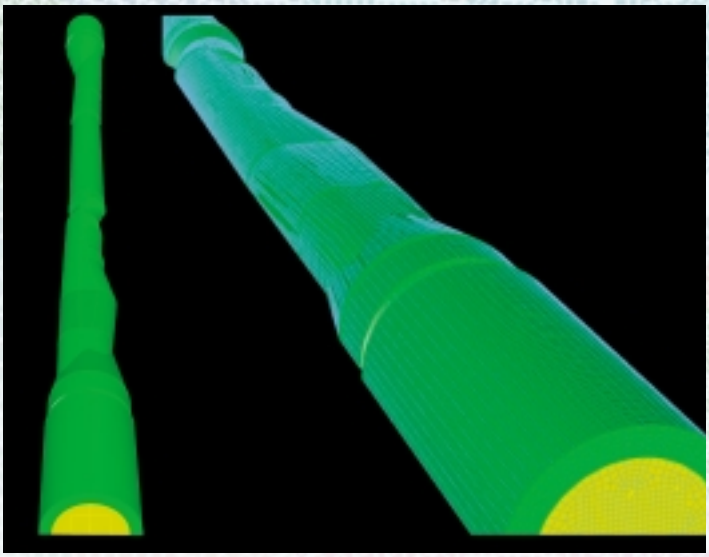
*Lori Freitag Diachin, SNL, (505) 284-9711, ladiach@sandia.gov*

*Jim Glimm, BNL and SUNY Stony Brook, (631) 632-8355, glimm@bnl.gov*



*Computed solution to the four-contact Riemann problem demonstrates the promise of high-order, adaptive Discontinuous Galerkin techniques for SciDAC astrophysics test problems.*



*TSTT delivers high-quality hexahedral meshes for the 21st Century Accelerator Science and Technology Center.*

Pacific Northwest National Laboratory

Oak Ridge National Laboratory

Rensselaer

Brookhaven National Laboratory

Argonne National Laboratory — University of Chicago

Sandia National Laboratories

Stony Brook — State University of New York


This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.